O,o'-biphenol, 4,4',6,6'-tetrafluoro-

Inchi: InChI=1S/C12H6F4O2/c13-5-1-7(11(17)9(15)3-5)8-2-6(14)4-10(16)12(8)18/h1-4,17-18H
InchiKey: JCEXUHNTCRBQDT-UHFFFAOYSA-N
Formula: C12H6F4O2
SMILES: Oc1c(F)cc(F)cc1-c1cc(F)cc(F)c1O
Mol. weight [g/mol]: 258.17
CAS: 388-14-7

Physical Properties

Property code	Value	Unit	Source
gf	-852.02	kJ/mol	Joback Method
hf	-1002.89	kJ/mol	Joback Method
hfus	37.25	kJ/mol	Joback Method
hvap	72.27	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.321		Crippen Method
mcvol	151.240	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
tb	705.56	K	Joback Method
tc	931.06	K	Joback Method
tf	553.72	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.04	J/mol×K	705.56	Joback Method
cpg	408.00	J/mol×K	743.14	Joback Method
cpg	416.48	J/mol×K	780.73	Joback Method
cpg	424.58	J/mol×K	818.31	Joback Method
cpg	432.43	J/mol×K	855.89	Joback Method
cpg	440.15	J/mol×K	893.47	Joback Method
cpg	447.85	J/mol×K	931.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C388147&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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